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A generalized theory of fatigue crack propagation in polymers is outlined. The theory accounts for fatigue crack propagation through root craze extension accompanied by simultaneous dissemination of microcrazing around the crack-root craze system thereby describing a crack-craze zone (CCZ). In addition to the conventional crack length, the width of CCZ is introduced as a new internal parameter. Applying a special

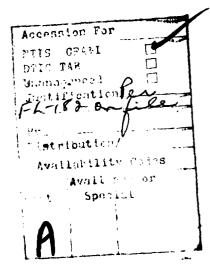
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version of the second law of thermodynamics: the principle of minimum thermodynamic forces, these internal parameters are formally described in terms of the reciprocal thermodynamic forces. The rate of crack extension per cycle was found to depend strongly on changes in the width of CCZ. Results of the model are applied to fatigue crack propagation data in polystyrene under various loading conditions and a good description of growth rates is observed.



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Technical Report No. 12

THE EFFECT OF MICROCRAZING ON FATIGUE CRACK / PROPAGATION IN POLYMERS.

BY

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INTRODUCTION

There has been a remarkable effort to elucidate the behavior of polymers under fatigue loading conditions. Recently, the phenomenology of polymer fatigue has been thoroughly reviewed by Hertzberg and Manson [1]. In analogy with the more well-studied low molecular weight materials, fatigue failure in polymers occurs due to the accumulation of damage resulting from repeated local plastic deformation. It is generally understood that the formation of crazes and associated cracks is responsible for the ultimate failure of many glassy polymers. However, the exact nature of the mechanisms involved is not yet well understood.

In view of the obvious importance that affiliates with the prediction of Fatigue Crack Growth (FCG) rates, various empirical as well as analytical approaches have been adopted in an attempt to develop the law of FCG. Conventionally, FCG "laws" are established by expressing the propagation rate of a starter crack in terms of the applied stress or a related function. It is not, therefore, surprising to find several such empirical "laws" in the form: $\hat{\ell} = f(K)^m$, where $\hat{\ell}$ is the rate of crack extension, K is the stress intensity factor, and m is a numerical factor.

As demonstrated by numerous examples in the recent literature, the conventional approach suffers from the lack of applicability to experimental data. This is due to the fact that these developments rest upon the classical view of fracture mechanics. That is, the failure process involves only the propagation of a single crack-cut; with or without a plastic

zone ahead of its tip. However, direct observations in polymers [2,3] and other materials [4] show that the crack propagates through a damage zone. Specifically, Bevis and Hull [3] have shown that the application of a tensile stress to a precracked specimen of polystyrene produced a halo of microcrazes surrounding the slowly growing root crack (Fig. la). A similar zone was also observed under low cycle fatigue of thin samples of polycarbonate and polystyrene [5]. The formation of a zone of microcrazes around the crack tip could be a source of substantial energy dissipation. This can be considered analogous to the classical crack-tip plastic zone. Clearly, a major alteration in the law of crack propagation would be expected due to this phenomenon.

In this paper, we present a more precise analysis of the problem of fatigue crack propagation. The treatment takes into account the role played by the microcrazing zone and its effect on the fatigue crack behavior under sinusoidal loading conditions. A more general expression of the failure process under such loading conditions is formulated. The model provides a good description of experimental data on the crack growth rate in polystyrene for which other models proved inadequate.

THEORETICAL DEVELOPMENTS

The Crack-Crazing Zone (CCZ): Based on the observations outlined in the introduction, failure processes in polymers, particularly under fatigue loading conditions, involved crack propagation, root craze extension, and the simultaneous spread of microcrazes around the crack-root craze (Fig. la). The "crack" system, thus described, is coined as "Crack-Craze Zone" and is abbreviated CCZ.

Along an axis perpendicular to the CCZ direction, microcrazing density assumes a bell-shaped distribution. However, for simplicity, the microcrazing distribution is approximated by an area of uniform microcraze distribution with a distinct boundary. The assumed boundary separates the microcrazed zone from the initial material (Fig. 1b). We consider CCZ propagation through a thin polymer sample so that two dimensional analysis may be applied and that isothermal conditions may be considered. Two geometrical parameters of CCZ are accounted for: length (ℓ) and width (ℓ) (Fig. 1b). Description of the CCZ history, therefore, requires the definition of the functions $\ell = \ell(t)$ and $\ell = \ell(t)$, where t stands for time.

Thermodynamics of CCZ Propagation: Viewed in thermodynamic terms, the propagation of CCZ is an irreversible process which is best treated by methods of irreversible thermodynamics. The thermodynamics potential G(Gibbs free energy) for the entire system can be expressed as the sum of two terms

 $G = G_1(\sigma, T, \ell, \alpha) + G_2(\sigma, T, \ell, \alpha)$ (1) G_1 and G_2 are the thermodynamic potentials of the CCZ and the complementary part of the body. The stress σ , and temperature, T, are external parameters, whereas ℓ and α are internal parameters.

Gibbs free energy, on the other hand, may be resolved into Helmholtz free energy of the initial material $F_{\rm O}(T)$, Helmholtz free energy of deformation F_{ϵ} (σ ,T) and the work A done by external forces. Therefore, we may write

$$G_{(k)} = F_{O(k)}(T) + F_{\varepsilon(k)}(\sigma, T) - A_{(k)}$$
(2)

k=1, 2 indicates the CCZ and the complementary part of the body, respectively. Because the total displacement \overline{u} may be considered as the sum of a reversible part (elastic) \overline{u}_e and irreversible (plastic) part \overline{u}_p which are associated with corresponding deformations ε_e and ε_p , the work A may be expressed as the sum of an elastic part and a plastic part, i.e.,

$$A_{(k)} = A_{e(k)} + A_{p(k)}$$
(3)

By definition, the potential energy (P) associated with the elastic deformation is given by

$$P_{(k)} = F_{\varepsilon(k)} (\sigma, T) - A_{\varepsilon(k)}$$
(4)

From (1), (2), (3) and (4) we obtain

$$G = F_{o_1} (T) + F_{o_2} (T) + P_1(\sigma, T, \ell, \alpha) + P_2(\alpha, T, \ell, \alpha)$$

$$-A_{p_1} - A_{p_2}$$
(5)

The entropy production rate due to propagation of the CCZ, as outlined above, is simply expressed as

$$T \dot{S}_{i} = \frac{\partial G}{\partial \ell} \cdot \ell + \frac{\partial G}{\partial \alpha} \cdot \alpha \tag{6}$$

Here, $\hat{\ell}$ and $\hat{\alpha}$ are the thermodynamic fluxes conjugated with the thermodynamic forces: $X_{\hat{\ell}} = \frac{-\partial G}{\partial \hat{\ell}}$ and $X_{\hat{\alpha}} = \frac{-\partial G}{\partial \alpha}$. These forces may be represented as follows

$$X_{\ell} = J + D_{\ell} - \gamma_{eff} \cdot \alpha$$
and
$$X_{\alpha} = M + D_{\alpha} - \gamma_{eff} \cdot \ell$$
 (7)

with $J=-\frac{\partial P_2}{\partial \ell}$ being the well known energy release rate, $M=-\frac{\partial P_2}{\partial \alpha}$ is a similar parameter which also has path-integral

representation for linear media. D_{ℓ} and D_{α} are the total dissipation energy rates associated with ℓ and α , respectively. An effective surface energy γ_{eff} consists of the sum of the difference between the free energy density of crazed and uncrazed materials (f_{02} - f_{01}), the crack surface energy density γ_{c} and the density of the potential energy of crazed material p_{1} , i.e.,

$$\gamma_{eff} = f_{o2} - f_{o1} + \gamma_c + p_1 \tag{8}$$

Generally γ_c is a negligible quantity in comparison to the free energy difference (f_{o2} - f_{o1}). Due to the small stress in the vicinity of the free edges of a crack, p_1 is also a small quantity.

Conventionally, the law of crack propagation is established by defining the relationship of the thermodynamic force X_{ℓ} , represented by stress intensity factor K, or the energy release rate J, and critical surface energy density γ , to the conjugated flux described as the crack growth rate ℓ . Because only one kinematic parameter is usually considered, i.e., ℓ , the constitutive law has been always approached by invoking the first law of thermodynamics (by satisfying the energy balance). When two or more kinematic parameters are considered, the energy balance alone would not suffice for the deduction of a constitutive law. In our case, where ℓ and α are considered, an additional principle is necessary. Therefore, a specific version of the second law of thermodynamics, that is, the principle of minimum thermodynamic forces [7], is considered.

In view of the second law of thermodynamics, the entropy production rate has to be non-negative. In the simple case of

 $\alpha = 0$, we can obtain from (6) and (7):

$$T \dot{S}_{i} = (J + D_{\ell} - \gamma_{eff} \cdot \alpha) \dot{\ell} \ge 0$$
 (9)

Consequently, the thermodynamic forces associated with crack growth rate ($\ell \geq 0$) must also be non-negative, i.e.,

$$J + D_{\ell} - \gamma_{eff} \cdot \alpha \ge 0$$
 (10)

Experimental observations of fracture surfaces [1] clearly show that crack propagates through the root craze by distinct jumps in a discontinuous fashion (discrete crack advance). Between jumps, damage within the craze fibrils accumulates until the system reaches a state of instability at which another jump occurs. Examination of the parallel discontinuous growth bands of many polymers indicates that a single jump approximates the length of a root craze. In this connection, it is believed that a new root craze evolves instantaneously past each jump.

Since both the energy release rate, J, and the effective surface energy $\gamma_{\mbox{eff}}$ depend only on CCZ configuration, therefore, they will not change between consecutive crack jumps where the system is considered stable. The dissipative energy, on the other hand, accumulates during load excursions. We may therefore, write:

$$D_{\mathfrak{g}}(\Delta \mathbf{N}) = \Psi(\ell, \alpha, \sigma, T) \cdot \Delta \mathbf{N}$$
 (11)

where Ψ is the energy dissipated per cycle and ΔN is the number of cycles per crack jump.

According to the second law of thermodynamics, crack may grow only when the condition (10) is satisfied, i.e.,

$$J + \Psi \cdot \Delta N - \gamma_{eff} \cdot \alpha \ge 0$$
 (12)

This expression describes necessary, but insufficient conditions of instability for the general case. Nevertheless, under the particular conditions considered, where a uniform stress is applied on the boundary of the system, (12) is necessary and sufficient. When instability is reached, i.e., equality of (12) is achieved, CCZ jumps into a new configuration, at which case

$$\Delta N = \frac{\gamma_{\text{eff}} \cdot \alpha - J}{\Psi}$$
 (13)

As we alluded to earlier, the length of a crack jump (Al) is considered equal to the length of the root craze. The average speed of CCZ propagation in the direction of the root crack is therefore given by:

$$\frac{\Delta \ell}{\Delta N} = \frac{\Psi \cdot \Delta \ell}{\Upsilon_{eff} \cdot \alpha - J} \tag{14}$$

In the following section, we proceed to evaluate the independent variables of this equation.

EQUATION OF CCZ PROPAGATION IN FATIGUE

A. Energy Dissipation in the Root Craze

In order to calculate the energy dissipation per cycle in the root craze Ψ , we introduce few modifications to the Dugdale model [8] which is illustrated in Fig. 2. In accordance with experimental observations indicating discontinuous crack growth [6], we suggest that the root craze does not undergo any significant propagation in the period between two crack jumps. During this period of no growth, the fibrils are assumed to be under a finite stress, distributed uniformly and defined as

 σ_* (t) \neq 0. The stress distribution assumed (Fig. 2) provides the following relationship between the crack length (l) and root craze (2b) in terms of external stress $\sigma_m(t)$ and $\sigma_*(T)$:

$$\frac{2b}{\ell} = 2 \sin^2 \left(\frac{\pi^* \sigma_{\infty}(t)}{4 \sigma_{\star}(t)} \right) \tag{16}$$

It should be noted that the formalism of the relationship (16) is identical to that derived by Dugdale [8]. However, the physical meaning of $\sigma_*(t)$ is different from that associated with σ_y in Dugdale's model as explained later in the discussion.

The microscopic evidence obtained from fatigue crack growth in many polymers justifies the assumption of a constant 2b/l ratio, within the period between two consecutive jumps. Accordingly, and from (16):

$$\frac{\sigma_{\infty}(t)}{\sigma_{*}(t)} = constant \tag{17}$$

For sinusoidal loading, the time dependent stress may be expressed as the following function:

$$\sigma_{\infty}(t) = \frac{\sigma_{\text{max}}}{2} [(1+R) + (1-R) \sin \omega t]$$
 (18)

where $R = \frac{\sigma_{min}}{\sigma_{max}}$ is the load ratio and ω is the load frequency.

From (17) to (18), we may write

$$\sigma_*(t) = \frac{\sigma_{*max}}{2} [(1 + R) + (1 - R) \sin \omega t]$$
 (19)

Here, σ_{*max} relates to the critical craze initiation stress which formally corresponds to Dugdale's σ_y . This stress is considered as the stress at which a "new" root craze initiates ahead of the crack at the moment of crack jump.

During a load cycle, the craze is believed to maintain the same geometry. Hence, the craze opening displacement is described by the following function:

$$\delta(\mathbf{x}, \mathbf{t}) = \delta_{\star}(\mathbf{t}) \cdot \phi(\mathbf{x}) \tag{20}$$

Here, δ_* is the opening displacement at the crack/root craze boundary (Fig. 2). The function $\phi(x)$ expresses the normalized distribution of the craze opening displacement along its axis and is equal to unity at the crack/root craze boundary. To account for the dissipation processes occurring within the craze material, it is reasonable to introduce a phase lag λ of the displacement $\delta_*(t)$ with respect to $\sigma_*(t)$. In accordance with equation (19), we may write:

$$\delta_*(t) = \delta_{*max^{\frac{1}{2}}} [(1 + R) + (1 - R) \sin (\omega t - \lambda)]$$
 (21)

From which the rate of crack/craze opening displacement is

$$\delta_{*}(t) = \delta_{*max} \cdot \frac{1-R}{2} \cdot \omega \cos(\omega t - \lambda)$$
 (22)

The dissipation energy per cycle Ψ of equation (11) can be given as:

$$\Psi = \int_{0}^{\pi/\omega} \int_{0}^{\pi/\omega} \sigma_{*}(t) \cdot \dot{\delta}_{*}(x,t) dx \cdot dt$$
 (23)

which upon integration yields:

$$\Psi = \beta_1 \quad \sigma_{*max} \quad \delta_{*max}$$
 (24)

The term β_1 of the above expression is given by:

$$\beta_1 = \frac{(1-R)^2}{2} \quad \sin \lambda \cdot \int_{0}^{\pi} \phi(x) dx$$
 (25)

In view of recent developments [9] in which the Dugdale crack opening displacement was derived in terms of the stress

intensity factor, we may similarly write:

$$\sigma_{*\max} \cdot \delta_{*\max} = \frac{K^2_{\max}}{E}$$
 (26)

Finally, the energy dissipation associated with the root craze per cycle can be given by

$$\Psi = \beta_1 \frac{K^2_{\text{max}}}{E} \tag{27}$$

B. Dependency of Crack Jump on the Stress Intensity Factor

We may recall that the crack propagates through the root craze by distinct jumps, each such jump is $\Delta \ell = 2b$ (the root craze length). From (16), and (17), it is obvious that $\Delta \ell$ is proportional to the crack length ℓ (Fig. 2). In fracture mechanics terms, the stress intensity factor is related to the crack length through the relationship: $K^2 = \sigma^2 \pi \ell$. $V(\ell/B)$, where the function V reflects the dependence of the stress intensity factor on the geometry of the specimen. B is a characteristic scale and is usually taken as the width of the specimen. Consequently, the crack length is given by

$$\ell = \beta_2 K^2_{\text{max}}$$
 (28)

where $\beta_2^{-1} = \sigma^2 \pi \cdot V(^{\ell}/B)$. As $\ell/B < 1$, the function $V(\ell/B - 1)$ and the crack length is proportional to K^2 .

Using equations (14), (25) and (26) and substituting $J = \frac{K^2_{\text{max}}}{E} \text{ , the equation of CCZ propagation may ultimately}$

take the form
$$\frac{\Delta \ell}{\Delta N} = \frac{\beta K_{\text{max}}^4}{E \cdot \gamma_{\text{eff}} \cdot \alpha - K_{\text{max}}^2}$$
(29)

where $\beta = \beta_1 \beta_2$.

DISCUSSION

The term $E.\gamma._{eff}$. α of equation (29) can be considered equivalent to the conventional critical stress intensity factor K_c^2 . Under conditions where α may vary during crack growth history, K_c^2 may become a history-dependent parameter.

Three distinct crack growth regimes can be recognized according to equation (29). The first regime is defined by $\frac{K^2}{K_c^2} << \text{ 1 at which case equation (29) can be rewritten as:}$

$$\frac{\mathrm{d}\ell}{\mathrm{dN}} = \frac{\beta K^{4}_{\mathrm{max}}}{K_{\mathrm{c}}^{2}} \left[1 + \left(\frac{K_{\mathrm{max}}^{2}}{K_{\mathrm{c}}}\right) + \ldots\right] \underline{\sim} \frac{\beta}{2} K_{\mathrm{max}}^{4}$$
(30)

Evidently, this regime is well approximated by Paris equation [11]. The condition $\frac{K^2}{K_c^2}$ $\stackrel{\sim}{}$ 1 defines the third regime in which

 $\frac{d\ell}{dN}$ vs. K^2 exhibits an asymptotic behavior (Fig. 3). Regime II can be quite complex as shown by the dotted lines in the figure. The complexity of this regime is strongly dependent on changes of α which may be envisioned negligible in regimes I and III as will be explained below.

Solution of equation (29) for two different values of $\alpha(\alpha_1 < \alpha_2)$ is represented in Fig. 4, where the strong dependence of the crack growth behavior on the magnitude of α is shown. It is therefore argued that the critical stress intenstiy factor, conventionally thought to be a material property, could be strongly dependent on the CCZ width and related changes. Such dependence has been established theoretically and experimentally for other materials [10]. In that report, $K_{\rm C}$ was found to be strongly dependent on the history of loading. It should be

emphasized here that the growth of α represents only one source for changing $K_{_{\rm C}}$. The evolution of another microcrazing zone far ahead from the CCZ constitutes another influential source to affect the magnitude of $K_{_{\rm C}}$. Naturally, the model proposed here can account for such diverse phenomena. During the crack propagation history, α changes into a higher value thereby causing a reduction in the crack propagation rate or even crack deceleration. This case is represented by the dotted line bridging the two constant α curves (Fig. 4). Such a plateau has been repeatedly observed in several materials including polymers under fatigue loading conditions. An example is shown in Fig. 5. The observed deceleration in crack growth strongly indicates the existence of a mechanism of energy absorption different from the main crack growth. Elucidation of such mechanism(s) is important for understanding factors governing material toughness.

APPLICATION TO DATA

As an illustrative test for the model, some fatigue crack growth data [12] are shown in Fig. 5 in the following form of equation (29):

$$\frac{\mathrm{d}\ell}{\mathrm{d}N} = \frac{\beta K^4_{\text{max}}}{K_c^2 - K_{\text{max}}^2} \tag{31}$$

Since the width of CCZ was not reported, the term K_c^2 has been approximated as an average of $3.0(\text{MPa})^2$.m from the recently accumulated data of polystyrene [13]. The dependency of β on R was estimated from the experimental data of figure 5. These values are tabulated below:

Inspite of the crude estimation made to evaluate equation (29), due to the absence of precise measurements of the related parameters, the model provides a reasonable description of the fatigue crack propagation. In a future publication, we report on more accurate measurements of the CCZ zone in various polymers together with further refinement of the model.

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FIGURE CAPTIONS

- FIG. 1 (a) Composite micrograph showing microcrazing associated with crack growth in polystyrene reproduced from ref. [3], and (b) Model of the crack-crazing zone (see text).
- FIG. 2 Crack-root craze configuration according to Dugdale model. Note that σ_* replaces σ_y of Dugdale.
- FIG. 3 An illustration of three-regime crack propagation history according to equation (29).
- FIG. 4 Crack propagation behavior at two different values of α . The dashes illustrates the transitional behavior when α changes into a larger configuration.
- FIG. 5 Fatigue crack propagation data for polystyrene taken from reference [12] and plotted in terms of the proposed model.

